

ALS

Modern Physics SH1012

Mattias Jönsson 940425-0673 matjon4@kth.se
Yue Jiao 911024-7799 yj@kth.se
2015-05-15

Introduction

One of the most important methods of studying properties of a material within modern physics is the spectroscopy. It is because that the spectroscopy of different atoms or molecules will too be different. However it is not that trivial how we get information from it. So we will demonstrate the theory and the method in this experiment. Here we shall try to determine the molecular vibrational constant and the Morse potential function of molecular iodine $I_2X^1\Sigma$ ground state. And then compare them to other people's result from reliable sources.

Theory

To study the vibrational property of the iodine in ground state we can use a laser with a certain wavelength to excite the molecule. In this experiment we use a NeHe 543.5 nm laser to excite the iodine from the ground state $I_2X^1\Sigma$ to the excited state $B^3\Pi_0$. This process shall happen because the energy of this wavelength of NeHe coincide with the difference of energy between there states. As a consequence of that, the molecule will jump back to lower energy levels, and release photons with specific energies **that correspond to those energy level**. And that can be observed by spectroscopy which we are using in this experiment. The result should be a characteristic spectrum consisting mainly of different peaks of detected photons for certain wavelengths.

To describe the shared potential of atoms in a two-atomic molecule, we can use the Morse function to approximate that. It is given by the equation

$$V(r) = D_e [1 - e^{a(r_e - r)}]^2$$

Here D_e is the dissociation energy in cm^{-1} . a is the Morse potential constant in \AA^{-1} . r is the interatomic distance in molecule and r_e is the equilibrium interatomic distance. they have units \AA .

And then we can solve the Schrödinger equation for this Morse function to get the quantized vibrational energy level E_v . For the ground state we have following relationship,

$$G(v) = \frac{E_v}{hc} = \omega_e \left(v + \frac{1}{2}\right) + \omega_e x_e \left(v + \frac{1}{2}\right)^2 + \omega_e y_e \left(v + \frac{1}{2}\right)^3, v = 1, 2, 3 \dots$$

Here ω_e , $\omega_e x_e$ and $\omega_e y_e$ are the rotational constants and v is the vibrational constant of the molecule.

And we know that that the energy corresponding to the wavelength of NeHe laser is going to excite the molecule to its state where $v = 26$. Then we will get another equation with different constant.

$$F(v) = T_e + \omega_e' \left(v + \frac{1}{2}\right) + \omega_e x_e' \left(v + \frac{1}{2}\right)^2 + \omega_e y_e' \left(v + \frac{1}{2}\right)^3, v = 1, 2, 3 \dots$$

With these two equations we can calculate the energy difference.

$$\sigma_v = \frac{1}{\lambda_v} = \frac{f_v}{c} = \frac{f_v h}{ch} = \frac{\Delta E}{hc} = F(v = 26) - G(v)$$

So, if we take the difference between two adjacent fluorescent emissions we will get

$$\Delta\sigma = \sigma_v - \sigma_{v+1} = [F(v = 26) - G(v)] - [F(v = 26) - G(v + 1)] = G(v + 1) - G(v)$$

Then we can define that

the energy of the photons correspond to the energy difference between the initial and final levels. Not to the energy of the final level

$$\Delta\sigma = \Delta G\left(v + \frac{1}{2}\right) = G(v+1) - G(v) = \omega_e - 2\omega_e x_e - 2v\omega_e x_e$$

We want to determine the vibrational constant v from the equation above. However the σ_v is observed in the experiment and the validity of equation. So one can conclude that the equation above is a linear equation of v . Therefore we can decide the ω_e and the $\omega_e x_e$ by plotting the observed value off differences $\Delta\sigma$ as a function of v .

If we calculate the sum of all the $\Delta D\left(v + \frac{1}{2}\right)$ for all v , we shall get an approximate of D_e which is following:

deltaG

$$D_e = D_0 = \frac{\omega_e^2}{4\omega_e x_e}$$

De=D0? What is the approximation?
Also, I do not see any sum in this equation. What was the mathematical approximation?

To find $\omega_e x_e$ we shall use the derivative of the Morse function and then we shall get:

$$\omega_e x_e = \frac{ha^2}{8\pi^2 c \mu}$$

Here h is the Plancks constant, c is the speed of light, μ is the reduced mass in unit kg which is

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

for a system of two objects

m_1 and m_2 here are masses of atoms inside the molecule and in our experiment the value if equal to the mass of the iodine atom.

And from literature we can find out that the rotation constant B_e can be expressed as following

$$B_e = \frac{h}{8\pi^2 c \mu r_e^2}$$

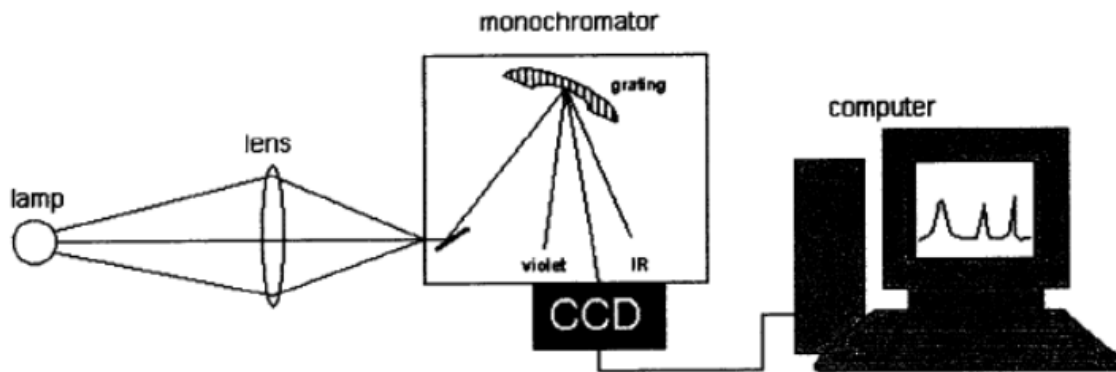
So at last we put all equation above together and we will be able to express ω_e and $\omega_e x_e$ with the observed statistics.

In the experiment part we can use ordinary lamp to measure the relationship between the wavelength of incoming light and the channel number inside the software we are using with the help of **grating** with known passing wavelength. The **grating** shall only let light with a certain wavelength pass.

filter

Experimental Setup

HeNe laser with wavelength 543.5nm	A test cell containing iodide, I_2
A focusing lens	A monochromatic Hg filters
A spectrometer	A computer for analyzing
Ordinary white light	



Step 1. Calibration CCD

We put a mirror in front of the SPE to reflex the light into it. Then we put a positive lens between the mirror and the SPE to gather the light. Now we start the software and check if there is a reading of anything. After we have gotten a reading we pause the software and put a grating just in front of the SPE so we can measure a new result. We adjust the ExpT which is the exposure time so we get a visible and sharp peak. We change the software to Peak Mode and take the value of the peak we find. When we find two peaks we record both. And we record also the wavelength corresponds to the peak which we already know. **For the second peak if there is one we use the wavelength times 2.** We measure four times channel number with four different gratings. And we get totally 7 relation between wavelength and channel numbers. We plot the result and get a linear relationship. And we calculate the first-degree polynomial to fit the relationship. The polynomial is needed later for measurement.

That is way too fast. I want you to explain what is the physical phenomenon happening. What is diffraction? A phase difference? Constructive/destructive interferences? How are the constructives interferences described, with which law? explain the law and how to use it

Step 2. Laser spectroscopy

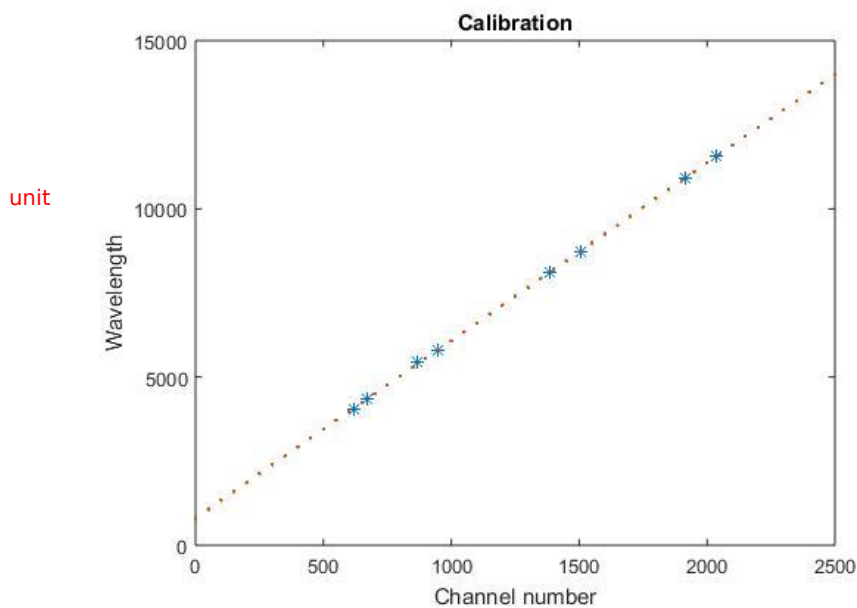
First we try to make the room as dark as possible. Then we start a HeNe laser and let it shoot through a container that contains iodine. We put a lens between SPE and the excited iodine cell and put a white paper at where the SPE stand. We move around the lens until we get a sharp picture of the laser on the paper. Then we remove the paper there and put a paper in front of iodine cell to block the light from laser. Then we change the software so it measures one time and then set that as background base. Then we change the software back to continue measuring and remove all papers and measure the laser by SPE. We get a graph with a lot of peaks and we record all of the channel numbers associate with ordinal number of the peaks. These are all the statistics we need. Now the experiment part is done.

Results

Part 1: Calibration

Wavelength [\AA]	4047	4358	5461	5780	8094	8716	10922	11560
Channel numbers	617	673	867	947	1387	1505	1913	2035

From this table we can calculate the relationship between the wavelength of incoming light and the channel number by doing the least square fit of those parameters, i.e. calibration. The figure is showed as following.



We will get that $\lambda = 5.2767c + 808.3531$ where c is the channel number.

Part 2: Spectroscopy

We can get the following peaks from the figure. And we can with the calibrated result to calculate the corresponding wavelength and the differences of wavelengths at the same time.

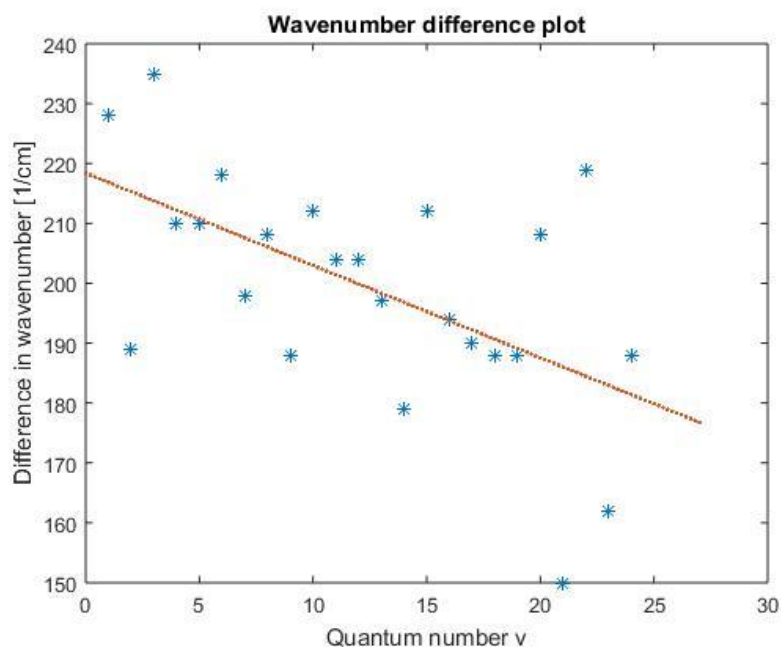
Channel	Wavelength [Å]	Differences of ^{wavenumbers} wavelength [$1\text{\AA}^{-1} = 10^8\text{cm}^{-1}$]	Missed channel
896	5420	2,28E-06	
909	5488	1,89E-06	
920	5545	2,35E-06	
934	5618	2,1E-06	
		2,1E-06	*
960	5754	2,18E-06	
974	5827	1,98E-06	
987	5895	2,08E-06	
1001	5968	1,88E-06	
1014	6036	2,12E-06	
1029	6114	2,04E-06	
		2,04E-06	*
1059	6271	1,97E-06	
1074	6349	1,79E-06	
1088	6422	2,12E-06	
1105	6511	1,94E-06	
1121	6594	1,9E-06	
1137	6678	1,88E-06	
		1,88E-06	*
1170	6850	2,08E-06	

1189	6949	1,5E-06	
1203	7022	2,19E-06	
1224	7132	1,62E-06	
1240	7216	1,88E-06	
1259	7315	-	

Here we get all the $\Delta\sigma$. We have put in several differences because of the Franck-Condon principle. This principle states that there are certain jumps between different states that are almost impossible. So there should be peaks at those places but it is not possible. We can add those imaginary peaks so the theory shall work. However we do not know precisely where to put those peaks than which channels these peaks should be between. So we choose the average of those two peaks lies at the side of them.

I asked during the lab for mathematics here. Prove me that peaks are missing (you can start from $\Delta G = \omega_e - 2\omega_e x_e(1+v)$). If you choose to do a linear interpolation, that is fine as long as you show me the approximations that are needed to do so. And to do that, you will have to show me some mathematics again.

We will get the following figure:



The linear fitting in this picture gives that the fitting equation is that

$$\Delta\sigma = -1.5404v + 218.3804 = \omega_e - 2\omega_e x_e - 2v\omega_e x_e$$

So we get

$$\begin{cases} -2\omega_e x_e = -1.5404 \\ \omega_e - 2\omega_e x_e = 218.3804 \end{cases} \Rightarrow \begin{cases} \omega_e x_e = 0.7702 \text{ units} \\ \omega_e = 219.9208 \end{cases}$$

So we find out that $\omega_e x_e = 0.7702 \text{ [cm}^{-1}\text{]}$ and $\omega_e = 219.9208 \text{ [cm}^{-1}\text{]}$.

With those values we can calculate the Morse function:

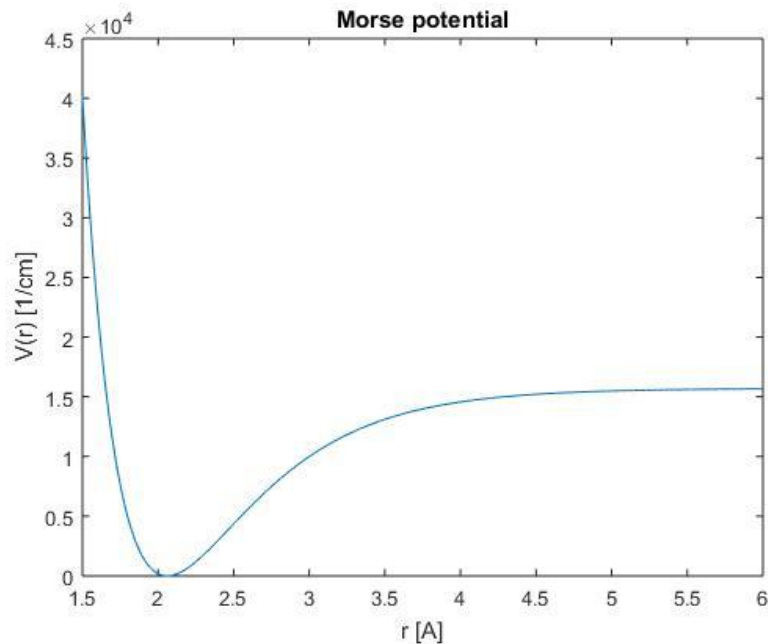
$$D_e = \frac{\omega_e^2}{4\omega_e x_e} \approx 15699 \text{ [cm}^{-1}\text{]} = 15700 \text{ [cm}^{-1}\text{]}$$

$$a = \sqrt{\frac{8\pi c \mu \omega_e x_e}{h}} \approx 1.70295 \times 10^{10} [\text{m}^{-1}] = 1.703 [\text{\AA}^{-1}]$$

$$r_e = \sqrt{\frac{h}{8\pi^2 c \mu B_e}} \approx 2.0607 \times 10^{10} [\text{m}^{-1}] = 2.061 [\text{\AA}^{-1}]$$

wrong unit
wrong value

Now we have all we need to calculate the Morse function $V(r) = D_e(1 - e^{a(r_e - r)})^2$. We shall get following plotting:



Conclusions

Here are all the values we are trying to find in this experiment.

$B_e [\text{cm}^{-1}]$	$\omega_e [\text{cm}^{-1}]$	$\omega_e x_e [\text{cm}^{-1}]$	$D_e [\text{cm}^{-1}]$	$a [\text{\AA}^{-1}]$	$r_e [\text{\AA}]$
3.127	219.9208	0.7702	15700	1.703	2.061

no. Take B_e from NIST

r_e is calculated without anything coming from the lab. A bit weird that your value is not the literature one's.

Discussion

We are overall satisfied with our results however there are some things that might be able to optimize.

First since the D_e is just an approximate of D_0 which is the value we need. So there shall be a small error but it is not so big since D_e is a quite good approximate.

how is it an approximation?

We think the biggest error source come from that it is hard to determine if a point is a peak or not. We think it is because that the room where we did the experiment was not dark enough. So the background noisy light was quite strong.

The background was strong, but it was not light. What was it?

References

Nist, 2015, <http://physics.nist.gov/PhysRefData/MolSpec/Diatomic/Html/sec6.html>

Also, your discussion is very lacking. Please think and comment on (at least but non limited to) the following points:

1. The birge Sponer approximation
2. The rotational levels
3. Your interpolation for the missing peaks
4. The angle of incidence of the photons
 - a. which is not the same during the caqlibration and the main part of the experiment. What does it mean for the calibration equation?
 - b. which is not the same for all the photons since the light is not perfectly collimated. What does it mean for the peaks and the results?